Explainable Network Growth by Folding on Typical Mis-predictions

Jimmy KANG

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- The black box nature of the training process weakens the **interpretability** of neural network models in understanding of the mechanisms behind their decision-making.

- The existing training strategy initializes **over-parameterized** models and allows representations to be learned in an anarchic manner from large amounts of data.
    - found to **underutilize the approximability** of the model
    - **decision criteria** are arranged in an unordered and susceptible manner

Related works

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Baseline: GradMax (Evci, et al., 2022)

GRADMAX: GROWING NEURAL NETWORKS USING GRADIENT INFORMATION

Utku Evci, Bart van Merriënboer, Thomas Unterthiner,
Max Vladymyrov, Fabian Pedregosa
Google Research, Brain Team
{evcu, bartvm, unterthiner, mxv, pedregosa}@google.com

ABSTRACT

The architecture and the parameters of neural networks are often optimized independently, which requires costly retraining of the parameters whenever the architecture is modified. In this work we instead focus on growing the architecture without requiring costly retraining. We present a method that adds new neurons during training without impacting what is already learned, while improving the training dynamics. We achieve the latter by maximizing the gradients of the new weights and efficiently find the optimal initialization by means of the singular value decomposition (SVD). We call this technique Gradient Maximizing Growth (GradMax) and demonstrate its effectiveness in variety of vision tasks and architectures[1].

1 INTRODUCTION

The architecture of deep learning models influences a model's inductive biases and has been shown to have a crucial effect on both the training speed and generalization (d'Áscoli et al., 2019; Neyshabur, 2020). Searching for the best architecture for a given task is an active research area with diverse approaches, including neural architecture search (NAS) (Elsken et al., 2019), pruning (Liu et al., 2018), and evolutionary algorithms (Stanley & Miikkulainen, 2002). Most of these approaches are costly, as they require large search spaces or large architectures to start with. In this

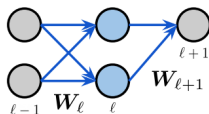# Baseline: GradMax (Evci, et al., 2022)
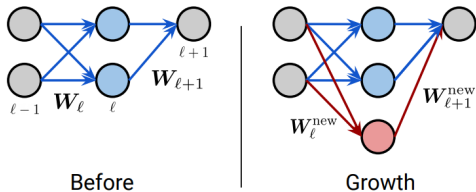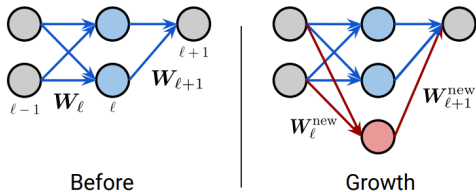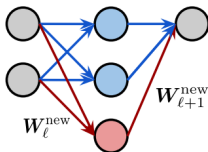

Before | Growth

Baseline: GradMax (Evci, et al., 2022)

Before | Growth

$$W_\ell^+ = \left[\begin{array}{c} W_\ell \\ W_\ell^{\text{new}} \end{array} \right]$$

$$W_{\ell+1}^+ = \left[\begin{array}{cc} W_{\ell+1} & W_{\ell+1}^{\text{new}} \end{array} \right] .$$

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Before

Growth
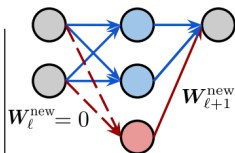
GradMax

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Before   Growth   GradMax
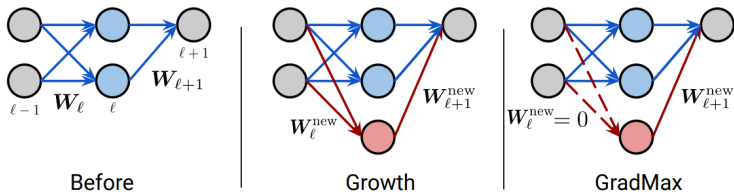
$$\underset{\boldsymbol{W}_{\ell+1}^{\text{new}}}{\arg\max} \left\| \boldsymbol{W}_{\ell+1}^{\text{new},\top} \mathbb{E}_D \left[\frac{\partial L}{\partial \boldsymbol{z}_{\ell+1}} \boldsymbol{h}_{\ell-1}^{\top} \right] \right\|_F^2, \quad \text{s.t. } \left\| \boldsymbol{W}_{\ell+1}^{\text{new}} \right\|_F \leq c.$$

Baseline: GradMax (Evci, et al., 2022)

Growing neural networks: When, where and how? Algorithms for growing neural networks start training with a smaller *seed architecture*. Then over the course of the training new neurons are added to the seed architecture, either increasing the width of the existing layers or creating new layers. Algorithms for growing neural networks should address the following questions:

1. **When** to add new neurons? For instance, some methods (Liu et al., 2019; Kilcher et al., 2019) require the training loss to plateau before growing, whereas others grow using a predefined schedule.

2. **Where** to add new capacity? We can add new neurons to the existing layers or create new layers among the existing ones.

3. **How** to initialize the new capacity?

In this work we mainly focus on the question of **how** and introduce a new initialization method for the new neurons. Our approach can also be used to guide when and where to grow new neurons. However, in order to make our comparison with other initialization methods fair we keep the growing schedule (**where** and **when**) fixed.

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Preliminaries - The Manifold Hypothesis

- DNNs can be seen as to approximate data distributions or decision boundaries by learning **manifolds** in high dimensional feature spaces (Bengio, Mesnil, et al., 2013; Bengio, Courville, and Vincent, 2013);

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Preliminaries - Growing DNNs Increase Non-linearity

Observation 1

Growing a DNN by adding new node(s) to broaden a specific layer introduces new dimension(s) to the latent feature space associated with that layer, which is, in nature, increasing the non-linearity of the low-dimensional projections of the manifold to enhances the network's capacity to model complex patterns.

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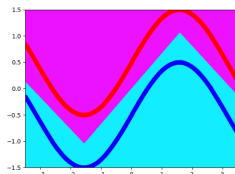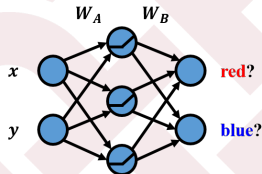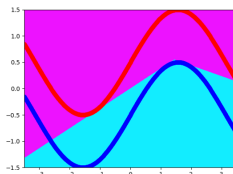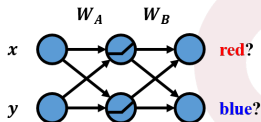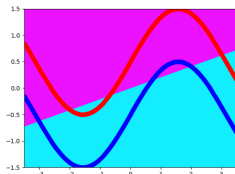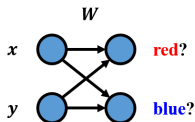
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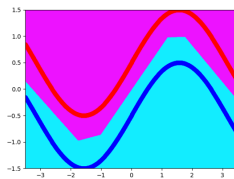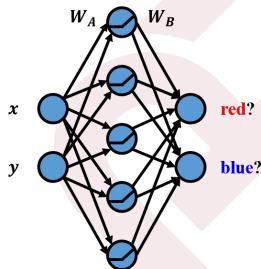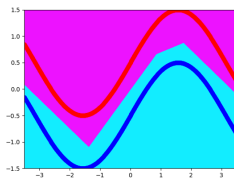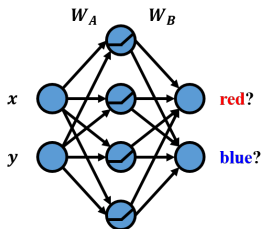
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4. Specifically, the model's capability (i.e., approximatability) can be increased by introducing non-linearity to its complexity,

5. which, can be achieved by breaking / folding the corresponding activated linear segment that leads to the typical mis-prediction.

Definitions

Definition (Activated Linear Segment)

For manifolds in high-dimensional spaces that are approximated by ReLU-based MLPs, their projections onto the input space are locally linear. In classification tasks, these projections are the decision boundaries, whereas in prediction tasks, they are the regression curves. Each piece of linear segments of these projections results from a composition of affine transformations governed by a specific activation pattern of ReLU units. These segments can thus be called "activated linear segments".

Definitions

Definition (Decision Boundary)

An $n-1$ dimensional hyper-plane on the n dimensional input space for distinguishing between two classes (the wrongly predicted class i given input and its ground truth class j), which is defined by equation $\vec{\boldsymbol{w}_{i-j}} \cdot \vec{\boldsymbol{x}} + b_{i-j} = 0$, where $\vec{\boldsymbol{w}_{i-j}}$ and b_{i-j} denote the differences between row i and row j of the affine transformation of the corresponding activated linear segment.

Definitions

Definition (Folding Crease)

An $n - 2$ dimensional sub-space on the $n - 1$ dimensional hyper-plane of the decision boundary that acts as the "transition line" between two contiguous activated linear segments, where the activation pattern changes.

Definition (Fold Point)

A single point $\vec{x_f}$ (an n dimensional vector) on the Folding Crease that can use for guiding the location of Folding Crease on the $n - 1$ dimensional hyper-plane of the decision boundary:

$$\begin{cases} \vec{w_{i-j}} \cdot \vec{x} + b_{i-j} = 0 \\ \vec{u} \cdot (\vec{x} - \vec{x_f}) = 0 \end{cases}$$ where $\vec{u}$ is a non-zero n dimensional vec-

tor that is orthogonal to the normal vector of the $n - 1$ dimensional hyper-plane of the decision boundary $\vec{w_{i-j}}$, i.e. $\vec{u} \cdot \vec{w_{i-j}} = 0$

Definitions

Definition (Typical Mis-predicted Instance)

Among all input data that is wrongly predicted by an model, the single input data instance that can be represents a certain kind of mistakes that the model cannot distinguish is called a "typical mis-predicted instance".

Determining Values for New Parameters

Theorem 3

Adding a Folding Crease on the Decision Boundary of an existing Acivated Linear Segment at a specific location $\vec{x_f}$ can be implemented by introducing a new node to the first layer of the shallow ReLU network and enfore the activation of its parameters (denoted as $\boldsymbol{w}_A^{\vec{new}}$ and b_A^{new} respectively) to occur exactly at point $\vec{x_f}$ using the equation $\boldsymbol{w}_A^{new} \cdot \vec{x_f} + b_A^{new} = 0$.

Notations & Symbols
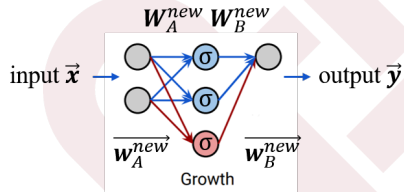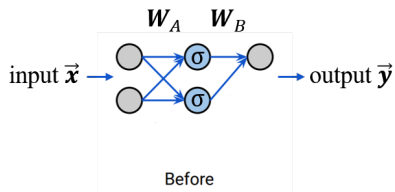
$$W_A^{new} = \begin{bmatrix} W_A \\ \overrightarrow{w_A^{new}} \end{bmatrix}$$

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Determining Values for New Parameters

Lamma 1

If and only if the $\vec{w_A^{new}}$ can be represented as an linear combination of $\vec{w_{i-j}}$ and $\vec{u}$ (i.e. there exist scalars α and β such that $\vec{w_A^{new}} = \alpha \vec{w_{i-j}} + \beta \vec{u}$), there is one and only one solution for variable b_A^{new} that for all input $\vec{x}$ on the Folding Crease, satisfy the above equation $\vec{w_A^{new}} \cdot \vec{x} + b_A^{new} = 0$.

Determining Values for New Parameters

Lamma 2

$$\frac{d\mathcal{L}}{d\vec{x}} = (\boldsymbol{W}_B \sigma(\cdot)' \boldsymbol{W}_A)^T \frac{d\mathcal{L}}{d\vec{y}} + (\boldsymbol{w}_B^{\vec{new}} \cdot \frac{d\mathcal{L}}{d\vec{y}}) \boldsymbol{w}_A^{\vec{new}}$$

Theorem 4

$\boldsymbol{w}_A^{\vec{new}}$ directly affect the direction of $\frac{d\mathcal{L}}{d\vec{x}}$ by specifying the direction of its component vector, while $\boldsymbol{w}_B^{\vec{new}}$ indirectly affect $\frac{d\mathcal{L}}{d\vec{x}}$ by determining the norm of its component vector.

Determining Values for New Parameters

Lamma 3

$\boldsymbol{w}_A^{\vec{new}}$ directly determines which input domains can activate the newly added node

Theorem 5

$\boldsymbol{w}_A^{\vec{new}}$ determines the location of the fold point after adding a new node.

Determining Values for New Parameters

Lamma 4

To ensure the affine transformation of the Activated Linear Segment does not vary much before and after introducing the new node, the parameters of the newly added connection in the second layer of the network model (denoted as $\vec{w_B^{new}}$) need to approach: $\begin{cases} \vec{w_A^{new}} \otimes \vec{w_B^{new}} \to \mathbf{0}_{n,n} \\ b_A^{new} \cdot \vec{w_B^{new}} \to \vec{\mathbf{0}} \end{cases}$ which can be further simplified as: $\min \|w_B^{new}\|^2$

Lamma 5

The above $\|w_B^{new}\|^2$ cannot be exactly equal to zero, otherwise no gradient can be backprogagated to update the corresponding parameters $\vec{w_A^{new}}$ and b_A^{new} in the first layer.

Proposed Method

Algorithm: Grow by Folding

---

initialize training dataset $\mathbb{X} = \{x_1, x_2, \ldots, x_n\}$, where $x_i \sim \mathbb{D}$ ($i \in \{1, 2, \ldots, n\}$, $\mathbb{D}$ is the input space)

initialize shallow ReLU MLP model f with parameters W_A, b_A, W_B, b_B

do loop: train f on $\mathbb{X}$ until converge

    find the most typical mis-predicted instance and a fold point on the decision boundary:

        $x_t, x_f = \textbf{fold\_point\_search}(\mathbb{X}, f)$, where $x_f \sim \mathbb{D}$

    calculate new parameters for the broaden model:

        $W_A^{new}, b_A^{new}, W_B^{new} = \textbf{hidden\_layer\_broaden}(x_t, x_f, f)$

    create new model and apply new parameters as initial values:

        $f_{W_A, b_A, W_B, b_B} \leftarrow f_{W_A^{new}, b_A^{new}, W_B^{new}, b_B}$

$f_{W_A, b_A, W_B, b_B} \leftarrow \textbf{equivalent\_network\_deepening}(f_{W_A, b_A, W_B, b_B})$

Proposed Method

Algorithm: Fold Point Search

---

input training dataset $\mathbb{X}$

input shallow ReLU MLP model $\boldsymbol{f}$ with parameters $\boldsymbol{W}_A, \boldsymbol{b}_A, \boldsymbol{W}_B, \boldsymbol{b}_B$

find the most typical mis-predicted instance:

$\quad \boldsymbol{x}_t = \textbf{find\_typical\_mis\_predicted\_instance}(\mathbb{X}, \boldsymbol{f})$

find the activated linear segment of model $\boldsymbol{f}$ given $\boldsymbol{x}_t$ as input:

$\quad \boldsymbol{W}_{activated}, \boldsymbol{b}_{activated} = \textbf{find\_activate\_linear\_segment}(\boldsymbol{x}_t, \boldsymbol{W}_A, \boldsymbol{b}_A, \boldsymbol{W}_B, \boldsymbol{b}_B)$

decision boundary regarding $\boldsymbol{x}_t$ can be defined by:

$\quad \{\boldsymbol{d}_1, \boldsymbol{d}_2, ..., \boldsymbol{d}_\infty\}$ s.t. $\boldsymbol{W}_{activated} \boldsymbol{x}_i + \boldsymbol{b}_{activated} = \boldsymbol{c}$, where $\boldsymbol{c}$ is a uniform vector

find the fold point $\boldsymbol{x}_f$ on the decision boundary that is closest to $\boldsymbol{x}_t$:

$$\boldsymbol{x}_f = \min_{\boldsymbol{d} \in \{\boldsymbol{d}_1, \boldsymbol{d}_2, ..., \boldsymbol{d}_\infty\}} \|\boldsymbol{d} - \boldsymbol{x}_t\|^2$$

output $\boldsymbol{x}_t, \boldsymbol{x}_f$

Proposed Method

Algorithm: Find Typical Mis-Predicted Instance

---

input training dataset $\mathbb{X}$

input shallow ReLU MLP model $\boldsymbol{f}$ with parameters $\boldsymbol{W}_A, \boldsymbol{b}_A, \boldsymbol{W}_B, \boldsymbol{b}_B$

sample subset $\mathbb{S} = \{\boldsymbol{x}_a, \boldsymbol{x}_b, ..., \boldsymbol{x}_m\}$ from $\mathbb{X}$

feed $\mathbb{S}$ into the model $\boldsymbol{f}$ and calculate their corresponding **values of loss function** $\mathbb{L} = \{l_a, l_b, ..., l_m\}$

performing **weighted k-means clustering** on $\mathbb{S}$ using corresponding $\mathbb{L}$ as weights and get clusters $\{\mathbb{C}_1, \mathbb{C}_2, ..., \mathbb{C}_k\}$

calculate average loss for instances in each clusters $\{l_{\mathbb{C}_1}, l_{\mathbb{C}_2}, ..., l_{\mathbb{C}_k}\}$

find the cluster $\mathbb{C}_i$ that has the highest average loss $l_i = \max(\{l_{\mathbb{C}_1}, l_{\mathbb{C}_2}, ..., l_{\mathbb{C}_k}\})$

find instance $\boldsymbol{x}_t = \min_{\boldsymbol{x}_i \in \mathbb{C}_i} \|\boldsymbol{x}_i - \boldsymbol{x}_c\|^2$, where $\boldsymbol{x}_c$ is the centroid of $\mathbb{C}_i$

output $\boldsymbol{x}_t$

Proposed Method

Algorithm: Hidden Layer Broaden

---

input typical mis-predicted point x_t

input fold point on the decision boundary x_f

input shallow ReLU MLP model f_{W_A, b_A, W_B, b_B} with parameters W_A, b_A, W_B, b_B

ensure $\forall x: W_B^{new} W_A^{new} x = W_B W_A x$:

   set $W_B^{new} = \begin{bmatrix} W_B & \mathbf{0} \end{bmatrix}$

   set $b_A^{new} = \begin{bmatrix} b_A \\ 0 \end{bmatrix}$

   set $W_A^{new} = \begin{bmatrix} W_A \\ w_A^+ \end{bmatrix}$ s.t.:

      ensure the grown new model fold only at point x_f:

$$W_A^{new} x_f + b_A^{new} = \mathbf{0}$$

      apply GradMax to W_A^{new}

$$\max_{W_A^{new}} \|\mathbb{E}_{\mathbb{D}} \nabla W_A^{new}\|_F^2$$

      align gradient direction with $W_A^{new}(x_t - x_f)$

$$\max_{W_A^{new}} \frac{\nabla W_A^{new} x_t \cdot W_A^{new}(x_t - x_f)}{\|\nabla W_A^{new} x_t\| \cdot \|W_A^{new}(x_t - x_f)\|}$$

output $W_A^{new}, b_A^{new}, W_B^{new}$

Supplementary Details

1. "Dead Layer" Problem

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   - Batch Normalization

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2. Optimization Problem of Fold Point Search Algorithm
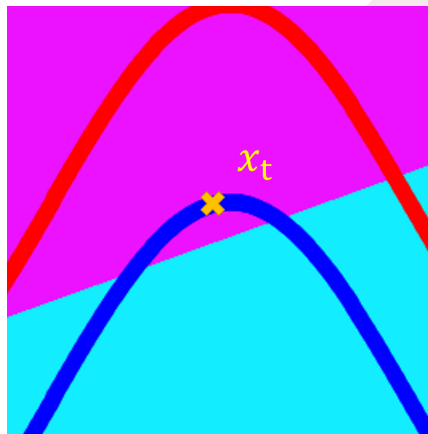
Supplementary Details
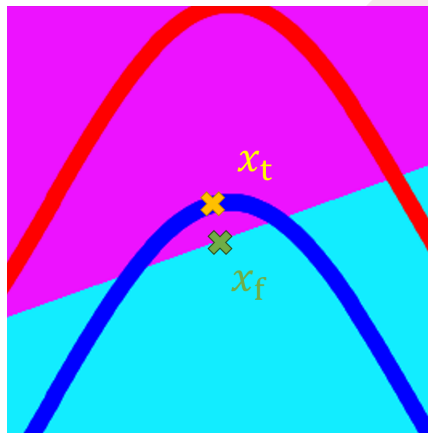
1. "Dead Layer" Problem
   - Batch Normalization

2. Optimization Problem of Fold Point Search Algorithm
   - given the equation of decision bondary: $w \cdot x + b = 0$, the closest point on the decision boundary can be found by
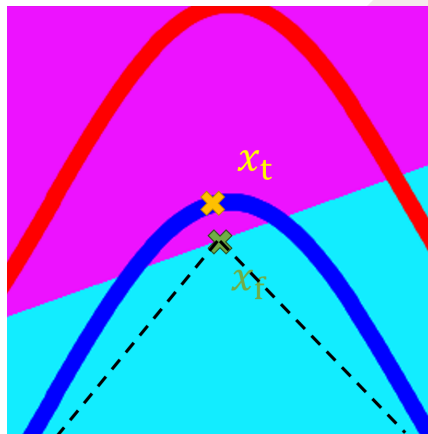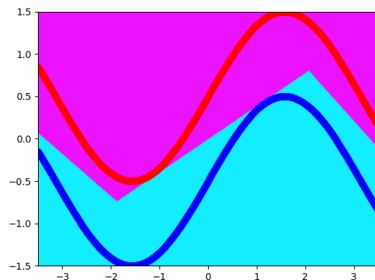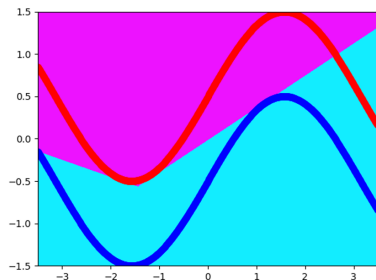 $x_t - ((w \cdot x_t) + b) * (w/(w \cdot w))$
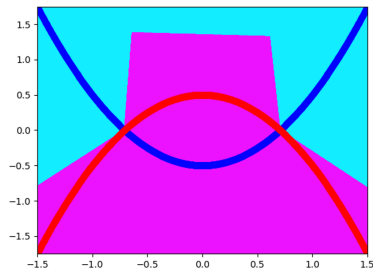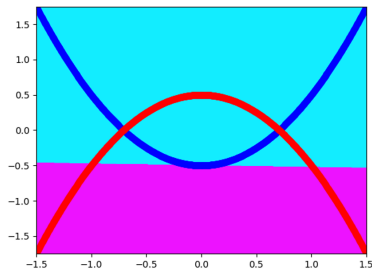
Example
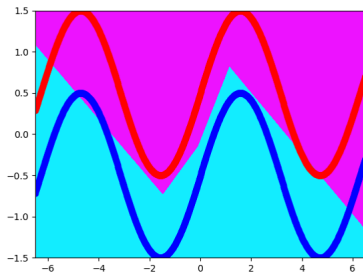
Example

Example

Binary Classification: Sine

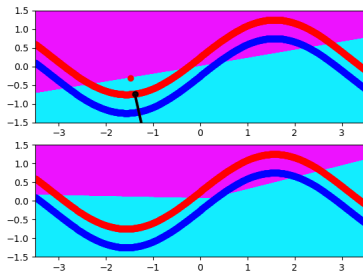# Binary Classification: Overlap Quadratic

Utilization of Approximatability

- random initialized: **65** / 1000
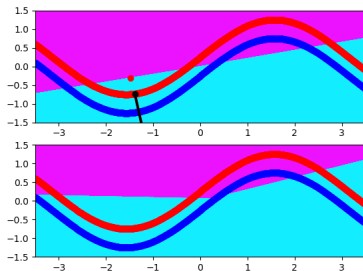- grow from 2-2-2 to 2-3-2: **360** / 1000

Next Milestones

1. due to the difference in updating speeds between the old and new parameters, the proposed direction along $\vec{x_t} - \vec{x_f}$ is not the most ideal gradient direction for updates

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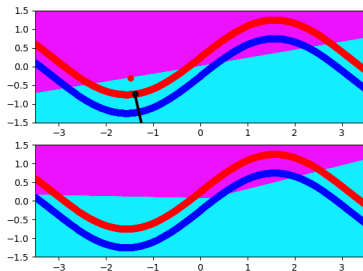
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3. Constrainted Optimization Difficulty

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Thank you!